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Title: (U) A Linear Response Model Predicts Reactivity From a Density Profile

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(U) A Linear Response Model Predicts Reactivity From a Density Profile

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Contents

1 Executive Summary

We tested the ability to predict the system reactivity, described by alpha, given a density profile using a simple linear system response. We generated a suite of 1-dimensional density profiles that consisted of nominal density, a discontinuity, and a decay. These profiles were prescribed a functional form and the mass was conserved in all cases. From these density profiles, we calculated the alpha value of the 3-dimensional system.

We calculated a linear response function given a training set of the 1-dimensional density profiles, and the system reactivity described by alpha. We tested the robustness of the response function using the remaining test data. Our results showed very good agreement between the predicted and calculated test values, where the distribution of alpha differences was centered about zero and had a standard deviation of 0.005 gens/shake. The predicted and calculated alpha values did not significantly differ ($t=-0.0009$ $p<0.99$).

We used Singular Value Decomposition (SVD) to reduce the matrix rank by retaining 95% of the cumulative singular value contributions. This reduced the matrix rank by 91.7%. We generated the linear response matrix and calculated the difference between the predicted and calculated alpha values. Using the reduced order matrix, we showed good agreement between the predicted and calculated alpha values where the distribution of differences was centered near zero, the standard deviation was 0.006 gens/shake, and the statistical t-test showed good agreement ($t=0.02$, $p<0.98$).

These results show a linear relationship between a series of 1-dimensional density profiles, where the mass was conserved, and the system reactivity. The next steps of this work will be to investigate the linear response using 2-dimensional density profiles.

2 Background

This study investigates the linear relationship between 1-dimensional density profiles and the reactivity of the 3-dimensional system. We sought to generate a response function from a training set of density profiles and utilize that response function to predict alpha for a testing set of density profiles.

3 Methods

We generated a series of 1-dimensional density profiles by systematically varying the parameters that define the profile. Then, we calculated the alpha values for each of the profiles. Finally, we solved for a linear response function to predict the alpha value given a density profile.

3.1 Density Profile Generation

We generated a suite of 1-dimensional density profiles that consisted of an initial density, a discontinuity, and a decay. These profiles were generated using the functional form as specified below. We first calculated an initial outer boundary radius based upon the mass

and initial density,

$$R_{b_0} = \left(\frac{M}{\frac{4}{3} \cdot \pi \cdot \rho_0} \right)^{(1/3)}, \tag{1}$$

where R_{b_0} is the initial outer boundary radius, M is the mass, and ρ_0 is the initial density. In all cases, the mass was 17000 grams and the initial density was 19.0 g/cc. Next, we calculated the discontinuity density, ρ_s, as,

$$\rho_s = \rho_b \cdot \left(\frac{R_s}{R_{b_0}} \right)^{-1/4}, \tag{2}$$

where ρ_b is the density at the outer boundary, R_s is the radius at which the discontinuity occurs, and R_{b_0} initial outer boundary radius defined in Equation 1. After the discontinuity, the density decayed by a power law, defined by,

$$\rho(r) = \left[1 - \frac{r - R_s}{R_b - R_s} \right]^{\gamma} (\rho_s - \rho_b) + \rho_b, \tag{3}$$

where R_s is the radius at which the discontinuity occurs, R_{b_0} is the initial outer boundary radius, γ is the power law, ρ_s is the density at the discontinuity, and ρ_b is the density at the boundary. The mass of the profile was conserved to 17000 grams in all cases by calculating a final outer boundary radius, R_b.

We generated 4900 cases, varying the density at the outer boundary, ρ_b; the power law, γ; and the discontinuity radius, R_s, as shown in Table 1. A plot showing some example

Table 1: The range of parameters that were used to generate a suite of density profiles.

Parameter	**Value Range**
ρ_b	19.0–20.0
γ	1.0–1.5
R_s	0.01–0.99

1-dimensional density profiles is shown in Figure 1.

3.2 Alpha Calculation

We used the 1-dimensional density profiles to generate 3-dimensional objects in MCNP6 [1] and calculated k_{eff} for each of the density profiles. The cases were sorted such that when k_{eff} was greater than 1.02, we ran the acode in MCNP6 to calculate alpha. For cases where k_{eff} was less than 1.02, we used a 14.1 MeV neutron source and tallied the number of neutrons leaving the outermost surface as a function of time. Alpha was calculated by differentiating the tally by the time steps, $\frac{1}{n}\frac{dn}{dt}$, the resulting noisy signal was smoothed using a moving boxcar of width 4, and alpha was calculated at 3 shakes after source injection.

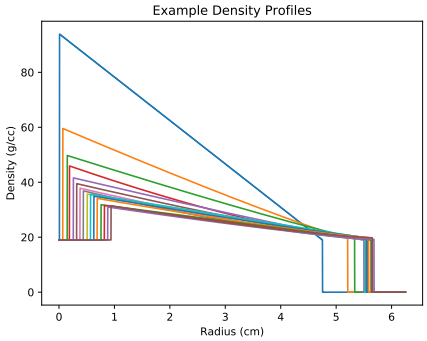


Figure 1: Examples of some 1-dimensional density profiles.

3.3 Response Function Calculation

The linear response function was calculated using the form,

$$\begin{bmatrix} \rho_1(r_1) & \rho_1(r_2) & \dots & \rho_1(r_m) \\ \rho_2(r_1) & \rho_2(r_2) & \dots & \rho_2(r_m) \\ \vdots & \vdots & \ddots & \vdots \\ \rho_n(r_1) & \rho_n(r_2) & \dots & \rho_n(r_m) \end{bmatrix} \begin{bmatrix} R(r_1) \\ R(r_2) \\ \vdots \\ R(r_m) \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{bmatrix}, \tag{4}$$

where the leftmost matrix contains the density profiles, the middle matrix is the response matrix, and the result is the matrix containing the alpha values. We solved this linear equation using 4700 density profiles to obtain the response function. Then we tested the result using the remaining 200 density profiles, multiplying by the response matrix, and calculating alpha.

In order to reduce the dimensionality of the system, we used Singular Value Decomposition (SVD) to reduce the rank of the data matrix. The principal components can be calculated by,

$$M = U\Sigma V^*, \tag{5}$$

where M is an $m \times n$ matrix, U is an $n \times n$ unitary matrix, Σ is an $n \times m$ rectangular diagonal matrix representing the singular values, and V is an $m \times m$ unitary matrix. The matrices U and V are orthogonal matrices that contain the orthonormal eigenvectors.

We reduced the rank of the matrix by taking 95% of the cumulative distribution function (CDF) of the singular values and recomputing the matrix, M,

$$M_{95} = U_{95}\Sigma_{95}V_{95}^*. \tag{6}$$

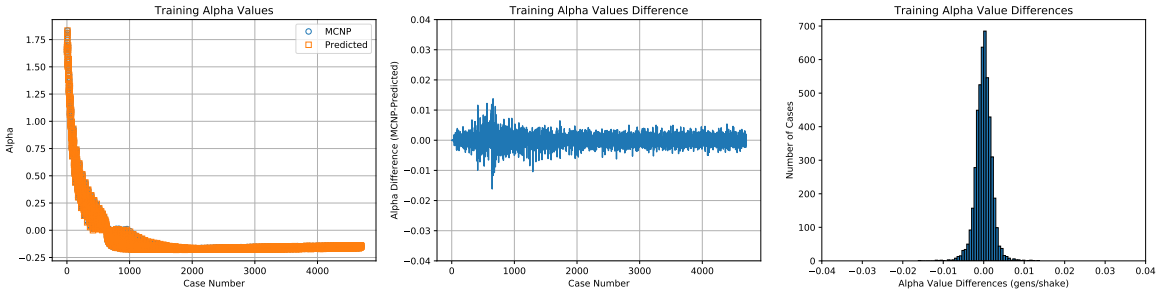
This reduced matrix representation of the data was used to calculate the linear response function. We tested the performance of the linear response function using the 200 test density profiles.

4 Results

We calculated the linear response function relating 1-dimensional density profiles with their calculated alpha value by solving Equation 4. We used 4700 randomly selected cases for calculating the response matrix and used the remaining 200 cases for testing the response.

4.1 Linear Response Function: Full Rank

In our initial assessment of this technique, we used the full rank matrix to calculate the response function. The predicted and calculated alpha values from the training data, along with the differences, are shown in Figures 2a and 2b. A histogram of the differences between

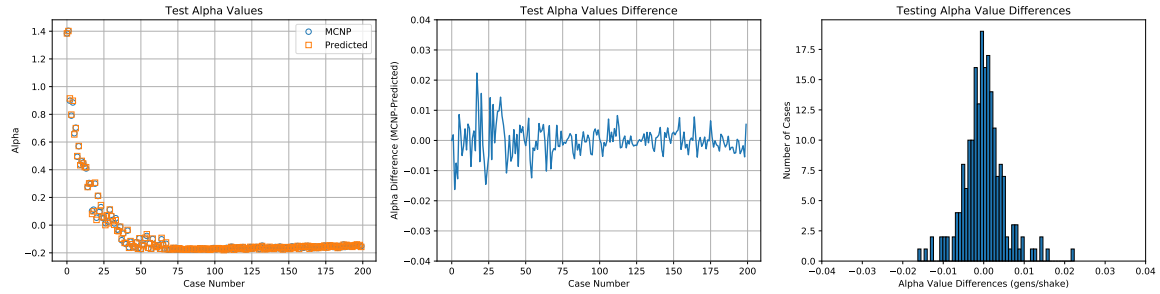


(a) Alpha Values **(b)** Alpha Differences **(c)** Alpha Diff. Distribution

Figure 2: The predicted alpha values from the full rank response matrix along with the alpha values calculated from MCNP using the training data.

the predicted and calculated alpha values are shown in Figure 2c. The deviations were centered around zero and had a standard deviation of 0.002 gens/shake. The predicted and calculated alpha values did not significantly differ (t=4.6e-7, p<0.99).

Using the test data cases, we investigated the feasibility of a linear response model to predict the alpha value given a 1-dimensional density profile. Figure 3 shows the predicted and



(a) Alpha Values **(b)** Alpha Differences **(c)** Alpha Diff. Distribution

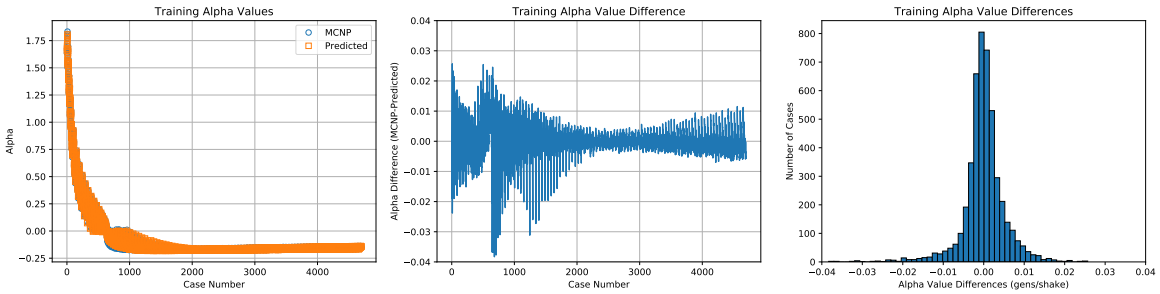
Figure 3: The predicted alpha values from the full rank response matrix along with the alpha values calculated from MCNP using the test data.

calculated alpha values from the test dataset. There was very good agreement in the alpha values from this linear response model. The difference between the predicted and calculated alpha values were centered around zero with a standard deviation of 0.005 gens/shake and the alpha values did not significantly differ (t=-0.0009 p<0.99).

4.2 Linear Response Function: Reduced Rank

Next, we sought to reduce the rank of the information matrix using SVD. We calculated the matrix, Σ from Equation 5 and plotted the CDF of the singular values. We retained values up to 95% of the CDF and discarded the remainder. This reduction utilized 8.3% of the principle components, thus significantly reducing the matrix redundancy. Using the remaining singular values and eigenvectors, we generated M_{95} as shown in Equation 6.

Using the reduced matrix, M_{95}, we calculated the response matrix as shown in Equation 4. The predicted and calculated alpha values, along with the differences, from the training data are shown in Figures 4a and 4b. A histogram plot of the differences in the predicted

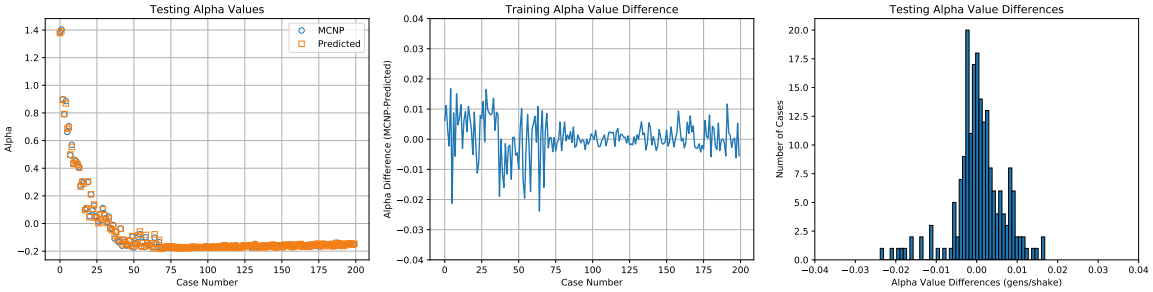


(a) Alpha Values **(b)** Alpha Differences **(c)** Alpha Diff. Distribution

Figure 4: The predicted alpha values from the reduced rank response matrix along with the alpha values calculated from MCNP using the training data.

and calculated alpha values is shown in Figure 4c. The distribution was centered about zero and the standard deviation was 0.005 gens/shake. The predicted alpha values did not significantly differ from the calculated alpha values (t=1.3e-5, p<0.99).

We tested the linear response matrix calculated using the reduced order SVD matrix. The predicted and calculated alpha values, along with the differences, are shown in Figures 5a and 5b. Figure 5c shows the distribution of differences between the predicted and calculated alpha values. The mean was centered around 0.0005 gens/shake with a standard deviation of 0.006 gens/shake. These results showed good agreement between the predicted and calculated alpha values using a response matrix generated from the reduced order training data matrix (t=0.02, p<0.98).



(a) Alpha Values **(b)** Alpha Differences **(c)** Alpha Diff. Distribution

Figure 5: The predicted alpha values from the reduced rank response matrix along with the alpha values calculated from MCNP using the test data.

5 Conclusions

We calculated the linear response matrix that, given a 1-dimensional density profile, could predict the system alpha value with very good agreement to the calculated alpha value. This study showed a linear relationship between a density field and the system reactivity.

In testing the response matrix, we showed that the distribution of differences between the calculated and predicted alpha values were centered about zero and had a standard deviation of 0.005 gens/shake. Overall, there was very good agreement between the predicted and calculated alpha values (t=-0.0009 p<0.99).

In order to reduce the rank of the matrix, we used SVD to retain 95% of the cumulative singular values. Using this reduced matrix, we calculated the linear response matrix. These results showed good agreement between the predicted and calculated alpha values where the distribution was centered near zero, the standard deviation was 0.006 gens/shake, and the predicted and calculated alpha values did not significantly differ (t=0.02, p<0.98). Reducing the matrix rank will be important when using 2-dimensional density profile data, which will square the matrix size for each case.

One source of uncertainty in these data arises from the two different methods used to calculate alpha. For density profiles where the k_{eff} value was greater than 1.02, the MCNP6 acode was used. In the remaining cases, a 14.1 MeV neutron was used to calculate the system reactivity. We observed slightly larger alpha differences when the system reactivity was near zero, primarily in the training data. This is likely due to the differences in the methods to calculate alpha. In real data, the neutrons are generated from photoneutrons and the distribution in the system is not symmetric. More realistic simulations, at a higher computational cost, may better simulate real data and reduce the uncertainty in the alpha predictions.

References

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